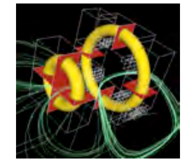


625-20-011

Project completion

A C++ Framework for Block-Structured Adaptive Mesh Refinement Methods

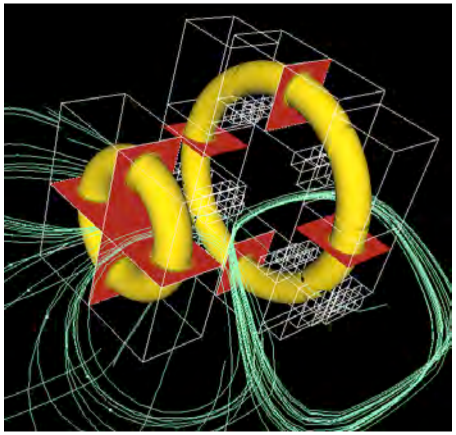
PI: Phil Colella, Lawrence Berkeley National Laboratory

A C++ Framework for Block-Structured Adaptive Mesh Refinement (AMR) Methods

PI: Phil Colella,Lawrence Berkeley National Laboratory

Objective

- Develop an object-oriented framework for enabling efficient block-structured adaptive mesh modeling applications on parallel and cluster computers with integrated visualization capabilities
- Provide computational technologies for multi-scale modeling of astrophysical and microgravity phenomena.



Adaptive mesh refinement (AMR) simulation of two co-rotating vortex rings (indicated by the yellow rings). The green lines show streamlines of the flow, while the white boxes show where finer resolution is used to better capture details of the flow.

Approach

- Baseline existing software framework for visualizing AMR data sets, known as Chombo-Vis
- Define capability requirements based on end user (microgravity and star formation) requirements
- Design and implement object classes and support libraries for multifluid and embedded particle applications
- Test and validate implementation against design requirements

Co-I's

Emily Nelson,NASA GRC

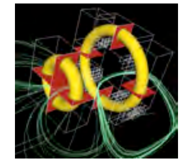
Key Milestones

• Initial design requirements defined with test plans specified	7/02
• First AMR implementation demonstrated with 5X reduction in time to solution	10/02
• Object Oriented classes and support libraries demonstrated for multifluid applications	6/03
• Demonstrate 5X reduction in time to solution for multifluid applications	11/03
• Demonstrate interoperability framework hosting both elliptic and hyperbolic solvers	6/04
• Completed package available via the Web	11/04

TRL_{in}=4

Colella, A C++ Framework for Block-Structured Adaptive Mesh Refinement (AMR) Methods

http://davis.lbl.gov/NASA/



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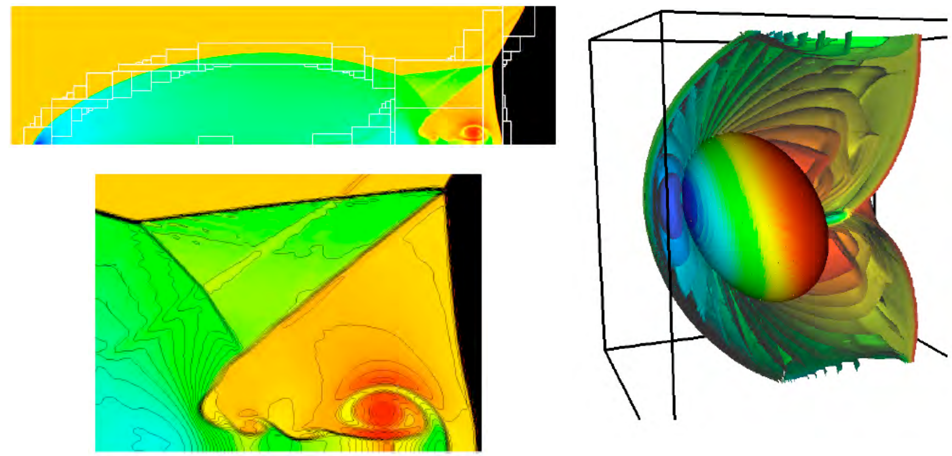


Chombovis AMR visualization tool examples in two and three dimensions

Accomplishments

- Fully documented high-performance C++ framework for developing adaptive mesh refinement algorithms (AMR) and particle methods
- State of the art AMR methods for gas dynamics, including a new unsplit PPM method.
- Scalable version of AMR code for hyperbolic conservation laws (scales to 1024 processors at 75 % efficiency)
- Scalable version of AMR code for incompressible flow (scales to 128 processors at 75% efficiency)
- New algorithms for simulating multiscale phenomena in astrophysics: AMR for MHD, self-gravitating gas dynamics.
- New algorithms for simulating multiscale phenomena in multiphase flow: second-order accurate method for suspended particles coupled to AMR for incompressible flow.
- Visualization and data analysis package for block-structured AMR data, including support for particles and material interfaces.

Impact *(see following 3 charts)*

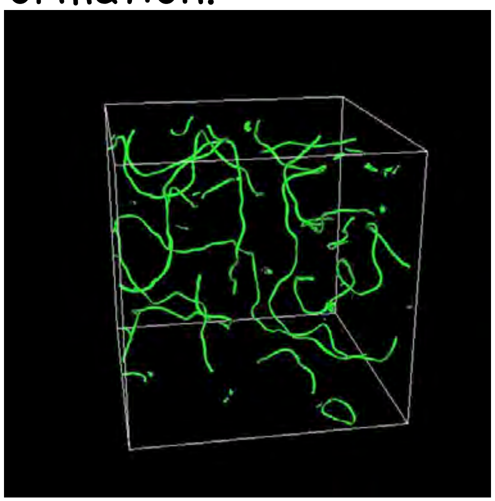
TRL=4_{in}-6_{out}

Applications Projects Using Chombo and ChomboVis Tools

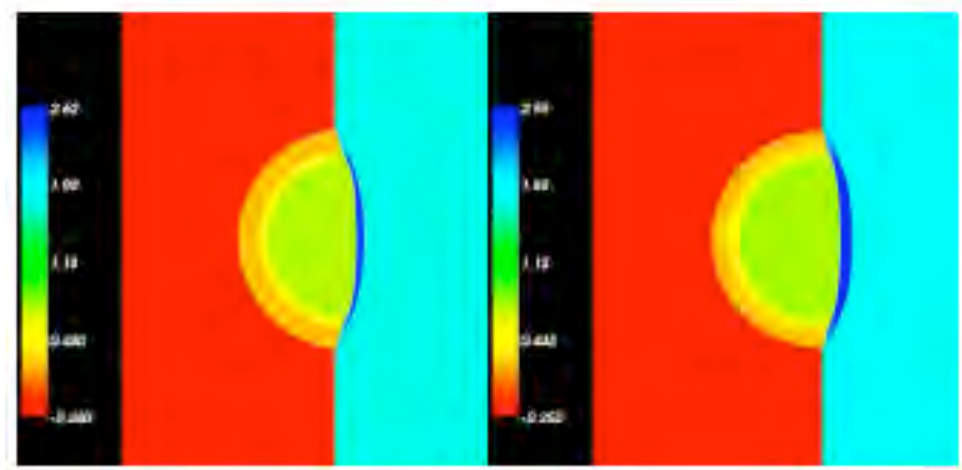
625-20-011

Chombo and ChomboVis development supported by NASA was coordinated with complementary activities in the DOE SciDAC program. The resulting software is being used in a variety of applications ranging from microbiology to cosmology.

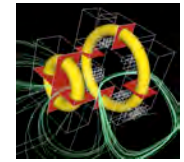
Astrophysics and Cosmology. Applications include semi-local string models for the early universe and gas dynamics with coupling to stiff cooling terms and particle models for collisionless matter for galaxy formation.



Second-order wave equation model of semi-local strings (joint with Julian Borrill, LBNL)



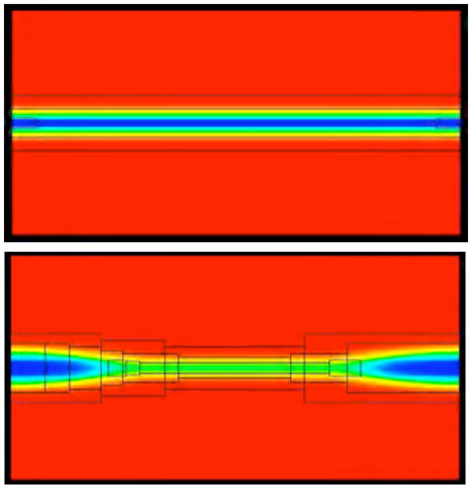
Shock-cloud interaction with radiative cooling. Left: stiff cooling. Right: marginally resolved cooling (joint with Francesco Miniati, ETH).

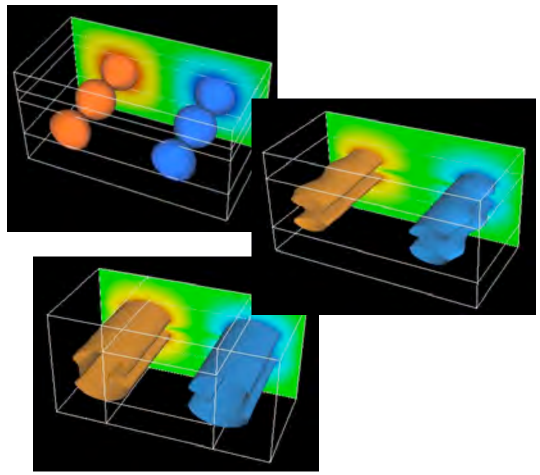


Applications Projects Using Chombo and ChomboVis Tools

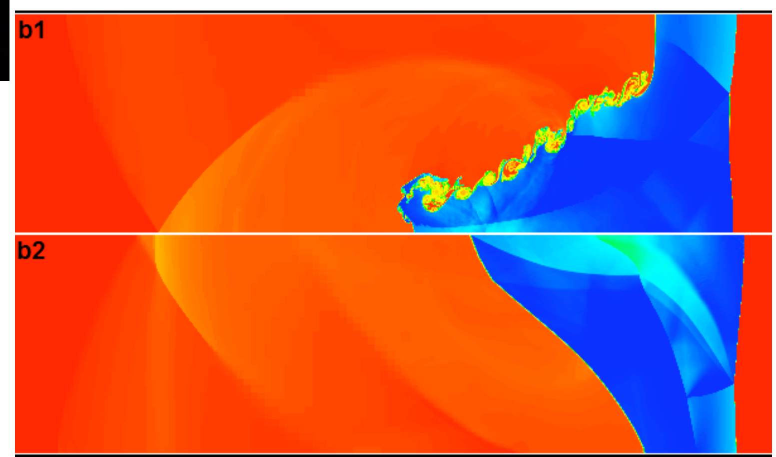
625-20-011

Magnetohydrodynamics. Developed models for ideal and nonideal MHD, used for fundamental investigations of plasma physics, as well as applications to magnetic fusion (joint with Ravi Samtaney, PPPL).

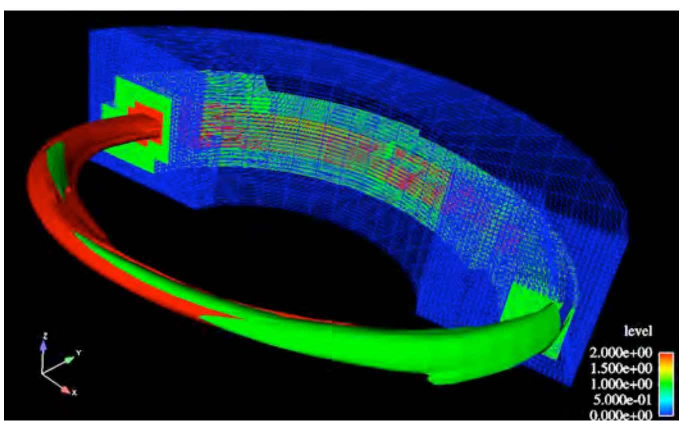




Magnetic reconnection, with nonideal physics leading to change in magnetic field topology. Left: 2D. Right: 3D.



Richtmyer-Meshkov instability (top) stabilized by applying a transverse magnetic field (bottom).

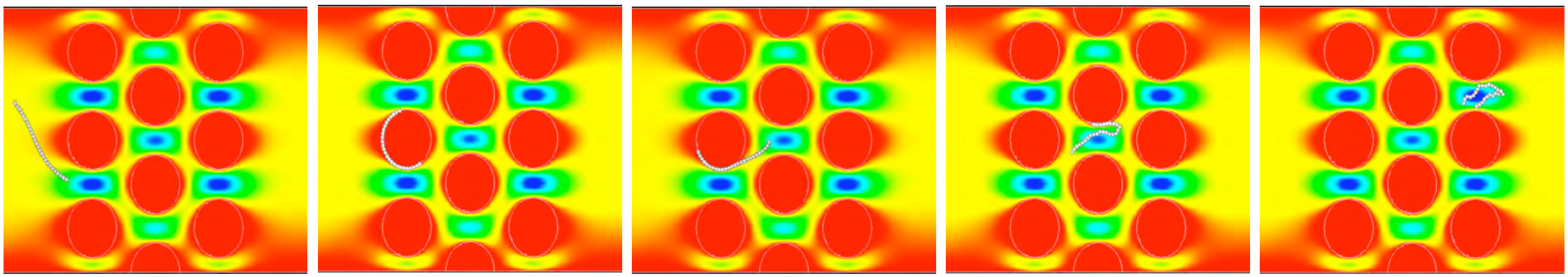


Simulation of pellet injection process for tokomak fueling .

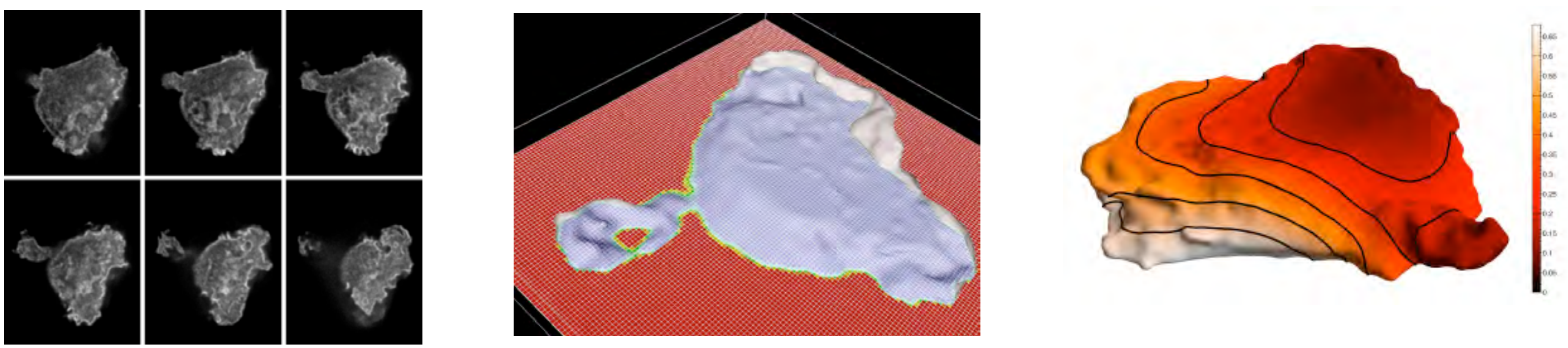
Applications Projects Using Chombo and ChomboVis Tools

625-20-011

Biology and Biotechnology. Models of microfluidics systems with fluid models coupled to particles representing polymers. Tools for representing biological systems in complex geometries using level sets.

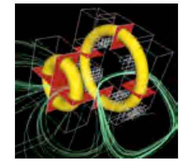


Time sequence of DNA transport. DNA molecule enters from left in frame 1, then wraps around bead in frame 2, is loosened by hydrodynamic and Brownian forces in frame 3 and is swept out of the chamber by the flow field in frames 4 and 5 (joint with David Trebotich (LLNL) and Gregory Miller (UC Davis)).



Modeling of reaction-diffusion processes in cells. Grey-scale confocal microscopy images (left) used to produce distance function representation of surface (center), leading to cut-cell representation of annular region for simulating diffusion on the surface (right) (joint with Adam Arkin, LBNL).

Achievement Quads



Colella, A C++ Framework for Block-Structured Adaptive Mesh Refinement Methods

http://davis.lbl.gov/NASA/

625-20-011

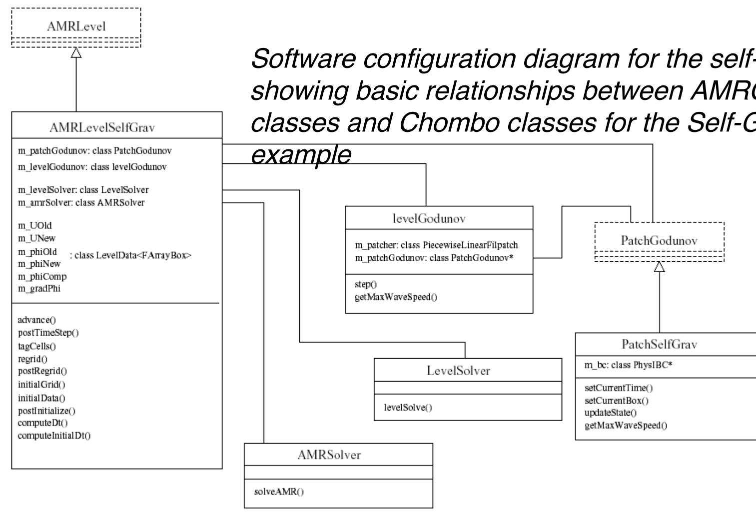
PI: Phil Colella, LBNL

Description

- Develop an object-oriented framework for enabling efficient block-structured adaptive mesh modeling applications on parallel and cluster computers with integrated visualization capabilities

Objective

- Computational technologies for multi-scale modeling of astrophysical and microgravity phenomena.



Software configuration diagram for the self-gravity code showing basic relationships between AMRGodunov classes and Chombo classes for the Self-Gravity example

Accomplishments

Developed eight key design and test documents

- Navier-Stokes with Particles Algorithm Design Doc
- Navier-Stokes with Particles Software Design Doc
- Navier-Stokes with Particles Test Plan Document
- Multifluid Algorithm Design Document
- Multifluid Software Design Document
- Multifluid Test Plan Document
- AMRGodunov (hyperbolic AMR) Design Document
- Hyperbolic AMR with Self-Gravity Design Doc

Key Milestones *(17 milestones total)*

- H - Initial design requirements defined with test plans specified — 7/02 (8/03)
- F - First AMR implementation demonstrated with 5X reduction in time to solution — 10/02
- I - OO Classes and support libraries demonstrated for multifluid applications — 6/03
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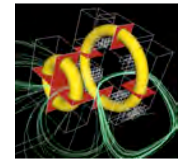
- K - Completed package available via the WWW — 11/04

$TRL=4_{in}-4_{current}$



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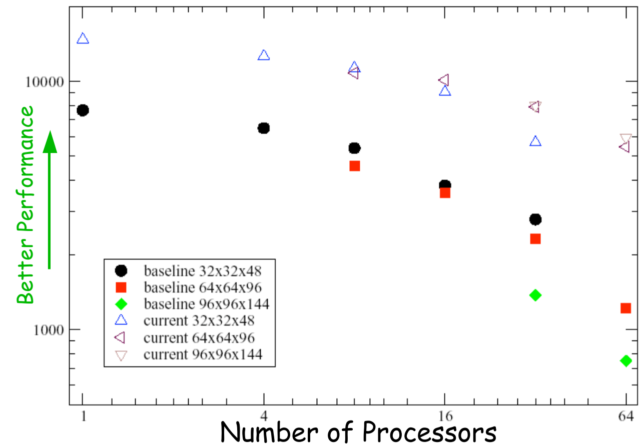
Performance:

$$\frac{\left(\frac{\text{Total number of points updated}}{\text{Wall-clock time}}\right)}{\text{Number of processors used}}$$



Accomplishments

- The benchmark is an incompressible AMR Navier-Stokes code running a problem with two co-rotating vortex rings in three dimensions.
- Performance and memory usage from baseline runs done on the Compaq AlphaServer SC45 at GSFC were reported in milestone E.
- Wall clock time was then reduced by factors ranging from 1.76 to 7.93, depending on the size of the problem and the number of processors.
- All performance improvements came from algorithm/code improvements, not from increasing the number of processors.
- Memory required was reduced by 5% to 20%.

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TRL=4_{in}-$4_{current}$

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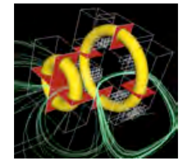

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Description
- Develop an object-oriented framework for enabling efficient block-structured adaptive mesh modeling applications on parallel and cluster computers with integrated visualization capabilities

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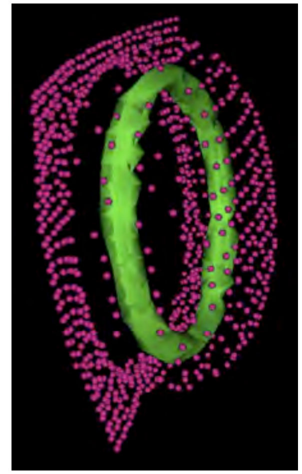
pyChomboVis visualization of a vortex ring interacting with suspended drag particles, the benchmark problem for the AMR Navier-Stokes code with particles code.



Accomplishments
Tested the interoperability prototype from Milestone H with improved codes:

- Extended the AMR incompressible Navier-Stokes code AMR-INS to support suspended particles in an incompressible fluid.
- Develop a hyperbolic AMR code for general systems of conservation laws based on unsplit Godunov / PPM methods.
- Updated the design and requirements documents. Baselined performance of the codes with the test suite from milestone H.

Key Milestones *(17 milestones total)*

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TRL=4_{in}-$5_{current}$

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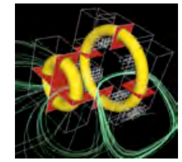

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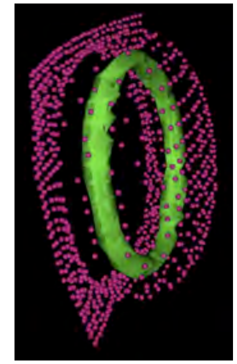
Large Problem Size	Large num processors	Scaled Efficiency
64x64x64	64	0.97
128x128x128	128	0.81



ChomboVis visualization of a vortex ring interacting with suspended drag particles, the benchmark problem for the AMR Navier-Stokes with particles code.

Accomplishments

Implemented algorithm and code improvements to the baseline AMR incompressible Navier-Stokes code "AMRINS with particles" code:

- Obtained scaled speedup with 81% efficiency on 128 processors for a vortex-ring problem with 32,768 particles.
- Compared to the baseline code:
  - Reduced wall clock execution time from a factor of 1.6 on 1 processor to a factor of 10.7 on 16 processors.
  - Reduced memory required from a factor of 2.3 on 1 processor to a factor of 7.7 on 16 processors.

Key Milestones *(17 milestones total)*

- H - Initial design requirements defined with test plans specified — 7/02 (8/03)
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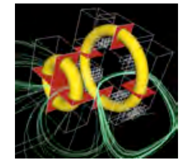

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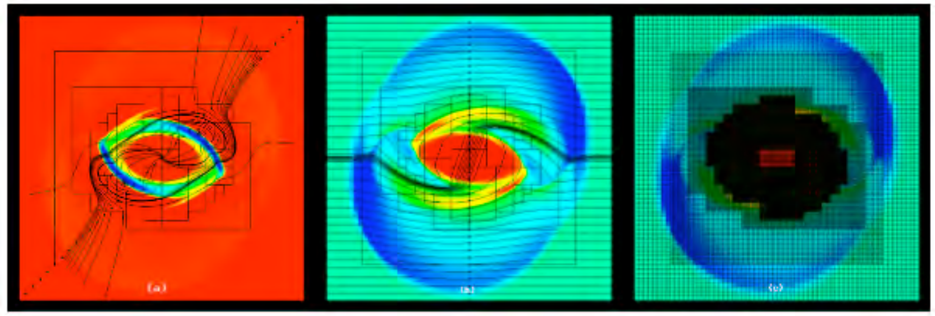

AMR MHD rotor problem

Accomplishments

- Coupled hyperbolic / elliptic solvers.
- Completion of AMR MHD capability.
- Completion of AMR gas dynamics with self-gravity capability.

Key Milestones *(17 milestones total)*

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G - Demonstrate 5X reduction in time to solution for multifluid applications 11/03 (2/05)

J - Demonstrate interoperability framework hosting both elliptic and hyperbolic solvers 6/04 (12/05)

K - Completed package available via the WWW (removed) 11/04

$TRL=4_{in}-6_{current}$

Computational Technologies